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Photonic MEMS for NIR *in-situ* Gas Detection and Identification

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Abstract—We report on a novel sensing technique combining photonics and microelectromechanical systems (MEMS) for the detection and monitoring of gas emissions for critical environmental, medical, and industrial applications. We discuss how MEMS-tunable vertical-cavity surface-emitting lasers (VCSELs) can be exploited for *in-situ* detection and NIR spectroscopy of several gases, such as O_2, N_2O, CO_x, CH_4, HF, HCl, etc…, with estimated sensitivities between 0.1 and 20 ppm on footprints ~10^{-3} mm^3. The VCSELs can be electrostatically tuned with a continuous wavelength shift up to 20 nm, allowing for unambiguous NIR signature determination. Selective concentration analysis in heterogeneous gas compositions is enabled, thus paving the way to an integrated optical platform for multiplexed gas identification by bandgap and device engineering. We will discuss here, in particular, our efforts on the development of a 760 nm AlGaAs based tunable VCSEL for O_2 detection.

I. Introduction

Gas analysis is typically carried out using laboratory analytical techniques, i.e. gas chromatography or mass spectrometry (GC-MS), which do not satisfy current device and material constraints for unattended, flexible ground sensors, or for lightweight, highly sensitive systems for avionic operations. IR absorption spectroscopy is the current alternative powerful approach for gas in-field detection and identification, and several interesting techniques have been developed including tunable diode laser absorption spectroscopy (TDLAS) [1]. Recently, micromechanically tunable vertical-cavity surface-emitting lasers (VCSELs) have been implemented in such fashion for NIR spectroscopy [2]. Unfortunately, many existing TDLAS systems exhibit drawbacks that limit their deployment including the need for cryogenic cooling, and a requirement for bulky multipass cells, or long hollow or porous fiber, with a relatively slow time response, [3]. We present the concept of a compact TDLAS extended to a miniaturized gas detection system utilizing MEMS-tunable optoelectronic devices.

This technology relies on an extended coupled cavity (ECC) MEMS-tunable VCSELs [4] in which the epitaxial materials structure is engineered to align the laser emission to a specific absorption wavelength (coarse tuning); additionally, these devices incorporate a micromechanically tunable optical cavity that allows for scanning of the emission wavelength over a wide and continuous range, allowing access to multiple absorption lines of the gas (fine tuning). In addition, when gases without a significant NIR signature are to be detected, complimentary techniques can be implemented on the same platform. Functionalizing the cavities with gas-sensitive coatings allows for enhanced detection through a change in the optical response of the coating (e.g. index shift, change in absorption, etc.). Resonant cavities with high quality factor (*Q*), amplify the magnitude of these changes. The details of this latter approach, particularly applied to H_2 sensing in an edge-emitting laser structure, are described in [5]. Finally, techniques including cavity ring down spectroscopy (CRDS) can be implemented to increase the sensitivity [6].

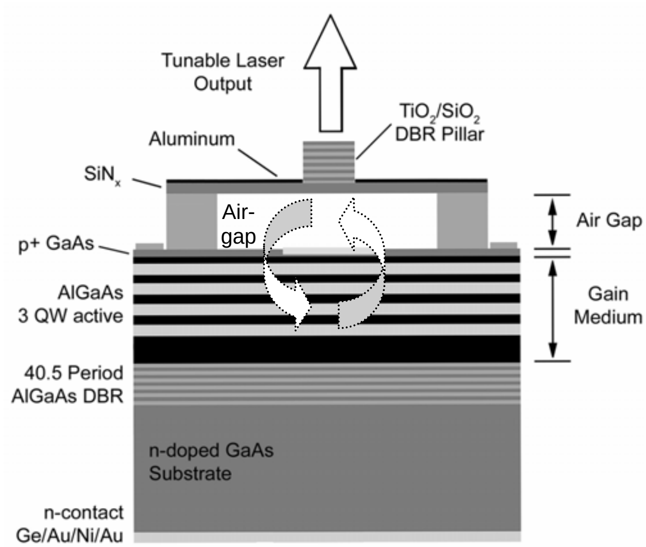

Figure 1. Cross-sectional schematic of the MEMS tunable ECC-VCSEL for O_2 sensing. The presence of gas in the air gap quenches the laser emission when the resonance wavelength is tuned to correspond with an appropriate absorption line.

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II. Device Design

The operation of the tunable-VCSEL-based gas sensor can be described as a multipass cell with optical gain. A sketch of this device is shown in Figure 1. In operation, the laser is electrically driven above threshold; the gas flowing through the air gap spoils the gain-loss balance necessary for lasing by increasing the absorption losses within the cavity. In this case the high-*Q* of the VCSEL structure enhances absorption as the light is reflected several (>100) times within the resonant cavity, between the top and bottom distributed Bragg reflectors (DBRs). During operation, the lasing power can be monitored remotely via transmission through an optical fiber or directly via an integrated detector.

A. Tuning Range and Sensitivity

In order to efficiently and selectively detect the signature absorption lines of the gas of interest, it is critical to design an appropriate tunable optical cavity. The absorption cross-section of O_2 around 760 nm is shown in Figure 2. (a). For our tunable VCSEL we desire the laser linewidth ($\delta\lambda$) to be < 1 pm within a full scanning range of at least 10 nm, an actuation voltage of < 10 V, and a power consumption on the order of tens of mWs. In Figure 2. (b) the threshold gain vs. wavelength is calculated showing the capability of continuous tuning over 20 nm within the wavelength range of interest. Dynamic mode-hop free tuning is inherent in MEMS-tunable VCSELs due to the extremely short axial cavity length. Thus, the wavelength resolution of the tunable laser is limited by the voltage source driving the electrostatic actuator, the stability of the micromechanical system, as well as the resolution of the read-out system.

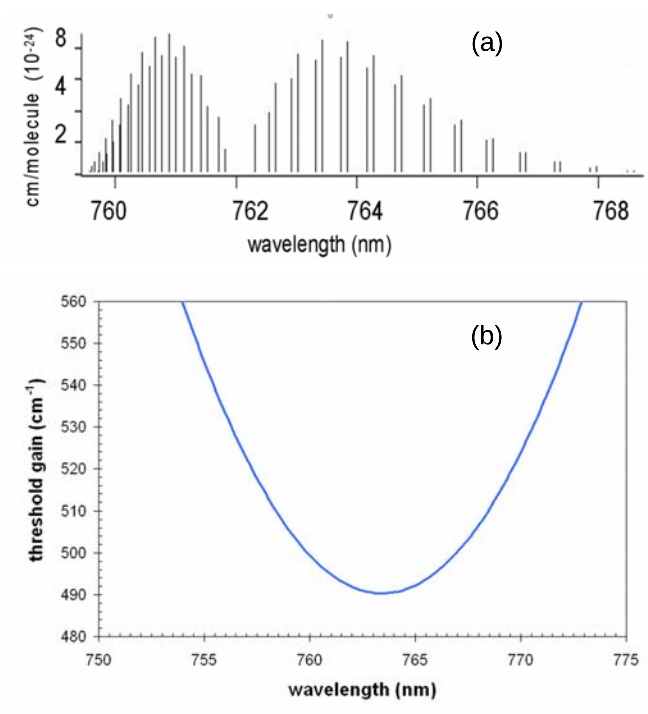

Figure 2. (a) Signature of O_2 at ~760- HITRAN source; (b) modeled laser threshold gain displaying continuous emission tuning for O_2 sensing.

The presence of gases in the VCSEL air gap affects the amplification factor or round trip enhancement of the power flow in the laser structure and thus the variation of output power when compared with the quiescent state P_o:

$$\frac{\Delta P}{P} = \frac{P_0 - P}{P_o} \propto \frac{A_0 - A}{A_o}. \tag{1}$$

The amplification factor in absence of any gas is given by:

$$A_0 = \left(1 - \exp(-\delta_g \mathrm{L}_{Cavity})\right)^{-1} \tag{2}$$

where $\delta_g = \alpha_0 - \Gamma g$ is the margin between the losses and the net modal gain of the laser [6][7]. Similarly to the Beer-Lambert law, the absorption of the chemical specie is accounted in *A* through the relative gas cross-section σ_{gas}:

$$\alpha_{gas}\left(cm^{-1}\right) = \sigma_{gas} C. \tag{3}$$

where *C is* the volume concentration of the gas specie. In such case δ_g becomes equal to $\alpha - \alpha_{gas} - \Gamma g$.

The limit of detection (LOD) of the sensor platform is determined by a combination of the device and read-out system sensitivity. In our initial evaluation we have taken into account the limited read-out system resolution by considering a conservative instrumentation resolution limit of $\Delta P/P = 10^{-3}$. An analytical analysis of the sensitivity of our lasers shows that for O_2 with a cross-section $\sigma_{NIR} \sim 10^{-21}$ cm^2/molecule (at room temperature and 1atm pressure), at the operation wavelength of 760 nm, an LOD ~ 20 ppm of volume in air can be obtained with a air-gap thickness of 5 μm. If we extend the analysis to other gases with higher NIR cross-sections, such as CO_x, CH_4, NO_x, HF, HCl, the LOD is very promising showing sensitivities to few ppm, as shown in TABLE I. For a tunable VCSEL with an air-gap thickness of 5 μm. For thicker air-gaps the sensitivity would increase.

TABLE I. Estimated Limits of Detection in the NIR

Gas	λ (μm)	σ (cm^2/mol)	LOD
O_2	0.76	10^{-21}	20 ppm
HF	1.27	10^{-19}	0.1 ppm
N_2O	1.38	10^{-21}	10 ppm
CO	1.57	10^{-21}	50 ppm
CH_4	1.65	10^{-20}	1 ppm
HCl	1.75	10^{-19}	0.1 ppm

B. Design and Fabrication of ECC VCSEL for O_2 sensing

Oxygen sensors are very important in controlling automotive and industrial emission processes for lower pollution and better yields, as well as improving flight safety. Concentration monitoring is also very important for biosensors in clinical diagnosis. These and fabrication motivations have induced us to focus our development efforts on tunable VCSELs optimized for O_2 sensors.

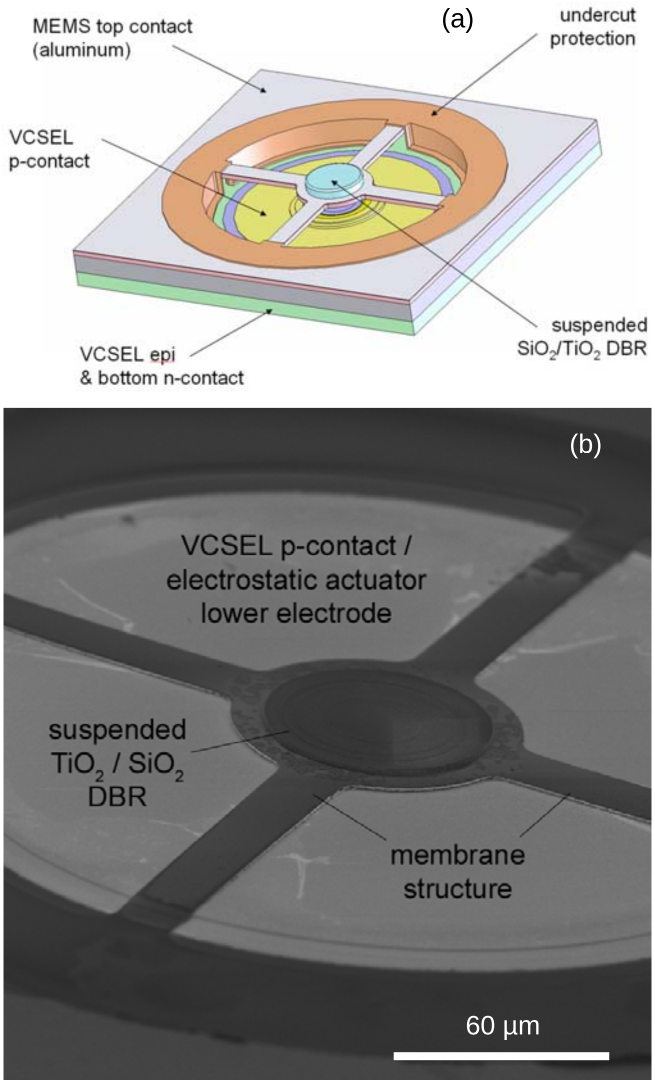

Figure 3. (a) 3-D model of the tunable VCSEL. Note that the scale of the air gap has been exaggerated to clarify the free-standing nature of the micromechanical structure. (b) SEM picture of tunable membrane.

Figure 3. display a solid model as well as a scanning electron micrograph of our tunable-VCSEL-based O_2 sensor. This device utilizes an identical mechanical design to wavelength tunable vertical-cavity semiconductor optical amplifiers (VCSOAs) demonstrated previously [8]. As opposed to the all-epitaxial devices from that research effort, the tunable mirror design discussed here incorporates an all-dielectric structure, consisting of a silicon nitride (SiN_x) membrane and an evaporated dielectric DBR. The use of the dielectric suspended mirror allows for the development of a platform-independent tuning mechanism that is capable of being integrated with various vertical-cavity laser and detector active materials including the III-P, III-Sb, and III-N materials systems. The flexibility in operating wavelength afforded by the use of low-temperature deposited dielectrics is useful for gas sensing applications where key absorption lines may span a region larger than that attainable by a single materials system.

For the tunable VCSEL, the suspended mirror structure is built atop a 760 nm AlGaAs “half-VCSEL” with a design similar to that outlined in [9]. A cross-sectional schematic of the tunable VCSEL is presented in Figure 1. The AlGaAs epitaxial structure consists of a 40.5 period bottom DBR—with linear composition grading between the high index ($Al_{0.30}Ga_{0.70}As$) and low index ($Al_{0.92}Ga_{0.08}As$) layers—and an active region incorporating three 8-nm $Al_{0.14}Ga_{0.86}As$ quantum wells (QWs) separated by 10-nm thick $Al_{0.40}Ga_{0.60}As$ barriers (band diagram depicted in Fig 4). The peak gain of the active region is designed to be near the absorption maxima of molecular O_2 in this wavelength range, as shown in Figure 4. Due to the strong absorption of the GaAs substrate, the VCSEL is constrained to be top-emitting, in this case through the MEMS-tunable mirror structure. Ohmic contacts to the VCSEL are provided by a Ti/Pt/Au p-contact annulus and a blanket deposited Ge/Au/Ni/Au contact on the backside of the n-doped substrate. Carrier and optical confinement are realized by non-selectively wet etching a shallow mesa and oxidizing an exposed $Al_{0.98}Ga_{0.02}As$ layer.

From the top down, the suspended mirror structure consists of an evaporated dielectric DBR (7 periods of TiO_2/SiO_2) on top of a tensile stressed (328 MPa) SiN_x structural film deposited via plasma-enhanced chemical-vapor deposition (PECVD). The combination of the TiO_2/SiO_2 stack and nitride membrane forms a 7.5-period DBR including the SiN_x layer as a high index quarter-wave layer. The tunable optical cavity utilizes the ECC design discussed in [4] and demonstrated most recently in [10]. In order to realize the extended cavity structure, a single film anti-reflection coating is included at the interface between the gain medium and air gap to eliminate coupled-cavity effects [11]. Including the large index discontinuity between the nitride membrane and air gap, the peak reflectivity of the top DBR is calculated to be 0.997.

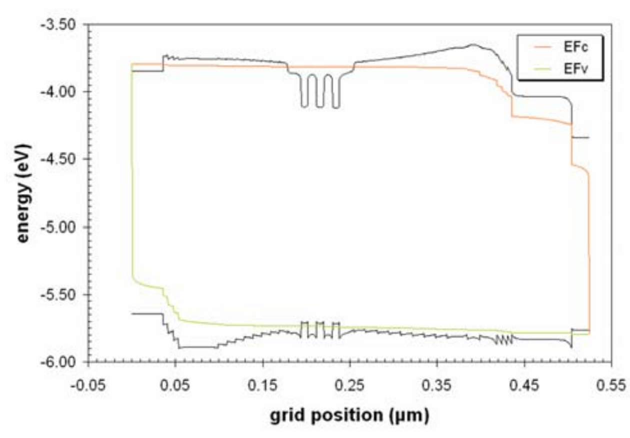

Figure 4. Band diagram of the VCSEL active region at 2 V bias.

For tuning of the emission wavelength, the device incorporates an integrated micromechanical actuator. An applied bias across the aluminum contact on top of the SiN_x structural film and the p-contact on the VCSEL mesa creates an electrostatic force that displaces the suspended mirror towards the substrate, reducing the optical path length and blue-shifting the resonance wavelength. As mentioned previously, because of the short cavity length of the VCSEL, wide and continuous single-mode tuning is possible in these devices. Previous demonstrations electrically injected tunable VCSELs utilizing the ECC-design (emitting within the telecom relevant wavelength range near 1550 nm) have demonstrated tuning ranges approaching 70 nm [10]. In this device, the use of the integrated electrostatic actuator allows for a rapid tuning response. Characterization of this micromechanical structure has demonstrated a near critically-damped response at atmosphere with a wavelength tuning time of < 10 μs [12]. As evident from Figure 3. we have developed a viable process flow for the tunable mirror structure and are now focusing on fabricating and characterizing these structures on 760-nm VCSEL epi-material.

C. *Future Direction*

For gases lacking significant NIR signatures, such as H_2, we can enhance the detection sensitivity by adding a gas-specific coating to the optical cavity. Here, it is critical to understand the appropriate coatings as well as their selectivity and specificity. Appropriate coatings include WO_3, SnO_2, PdO, ZnO, porous Si, for use in monitoring NO_x, CO, H_2S, Cl_2 etc. These coatings will exhibit changes in refractive index when exposed to the appropriate target gas species, resulting in a measurable wavelength shift in the laser output spectrum.

The basic technology outlined in this work is promising in that in can be extended to several material systems in the visible, as well as the short wavelength infra-red (SWIR) range (2-3 μm) where molecules have higher absorption cross-sections. Recent developments have led to the demonstration of micromechanically-tunable filter structures integrated with HgCdTe materials structures for widely tunable resonant detectors in this wavelength range [13]. Additionally, the technology has the potential of being extended to highly sensitive CDRS by integrating active (laser, detector) and passive devices (low loss filters) on the same platform [6].

III. CONCLUSIONS

Typically, samples are collected in the field and transported to the laboratories for analysis, i.e. GC-MS. We have instead proposed a compact tunable optical cavity for *in-situ* NIR spectroscopy. The MEMS-tunable VCSEL platform discussed in this work represents a solid foundation for a new class of compact, sensitive, and fiber compatible sensors for fieldable, real-time, multiplexed gas detection systems. LODs for gases with NIR cross-sections such as , O_2, CH_4, CO_x, NO_x, have been predicted to approximately span from 10ths to 10s ppm. We are currently focusing on oxygen detection for which we have developed a design and a process for 760 nm continuously tunable VCSELS. This technology can potentially lead to development of *in-situ* self-calibrating platforms with adaptive monitoring by exploiting our parallel efforts on Photonic FPGAs [14] .

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